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Modelling of Organic Aerosols...
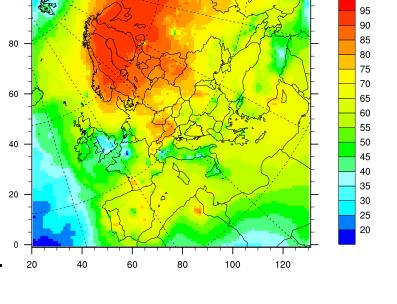
David Simpson

Norwegian Meteorological Institute

Activities 1: Emissions

- Revised BC/OC inventory for 2000, IIASA, Feb 2005

- 'EMEP' Time-series , SOx, NOx, OC, BC; 1890-2000. (Technology/fuel-based estimate)

- Independant estimate of wood-burning emissions (underway)

- Improved ship-emissions

Activities 2: SOA model

- Investigations of vapour pressure methodologies

- Implementation of new species (e.g. fulvic acids), following functional-group ideas

- Implementation of tracer species
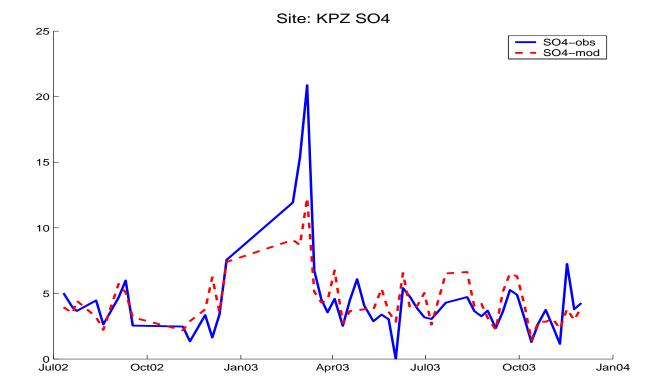
- Search for correlations/relationships

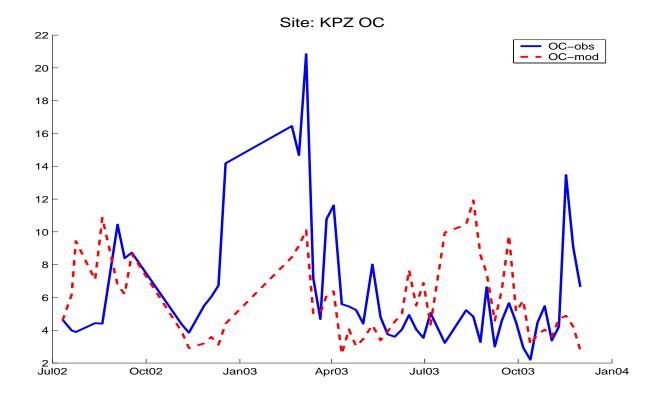BSOA/OC (%)

Activities 3: Other projects

- CARBOSOL (EU FP5)
  - Focus on southern/central Europe
  - 3 Years of data, including tracers (levoglucosan, ^{14}C, HULIS)
  - + ice-core data
- MISTRA (Sweden, with GU)
  - Combined measurement/modelling
  - e.g. Göte-2005 campaign
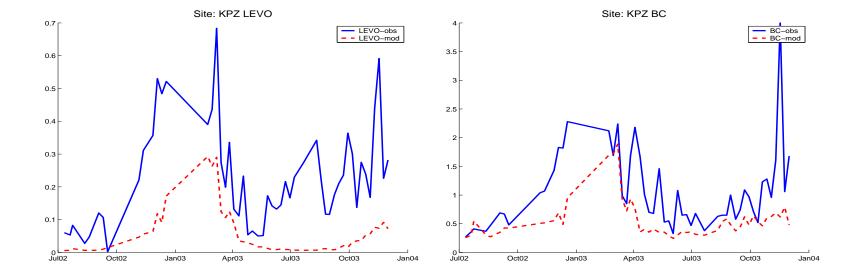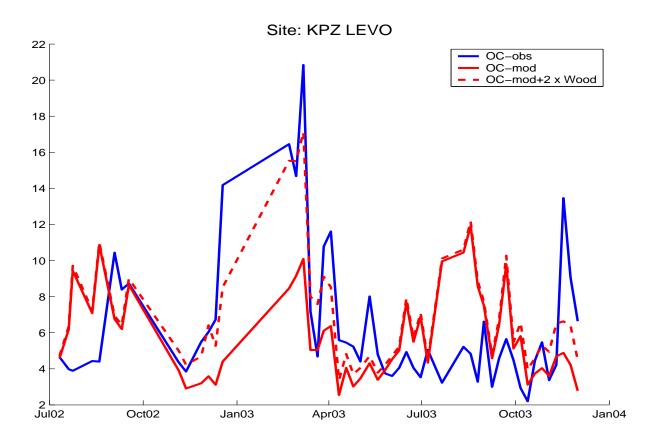 - Modelling focus so far on vapour pressure calculations

CARBOSOL Comparisons

Site: KPZ SO4

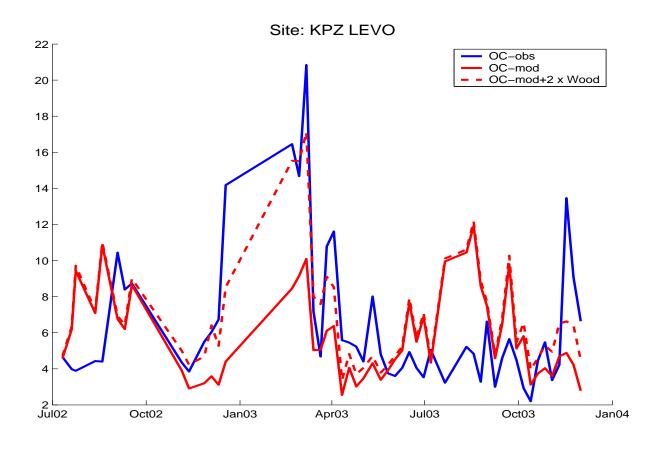# CARBOSOL Comparisons

Site: KPZ OC

CARBOSOL Comparisons

Wood burning?

Increase wood OC by factor 3:

Wood burning?

Increase wood OC by factor 3:

Site: KPZ LEVO

Legend:
- OC–obs
- OC–mod
- OC–mod+2 x Wood

Wood burning?
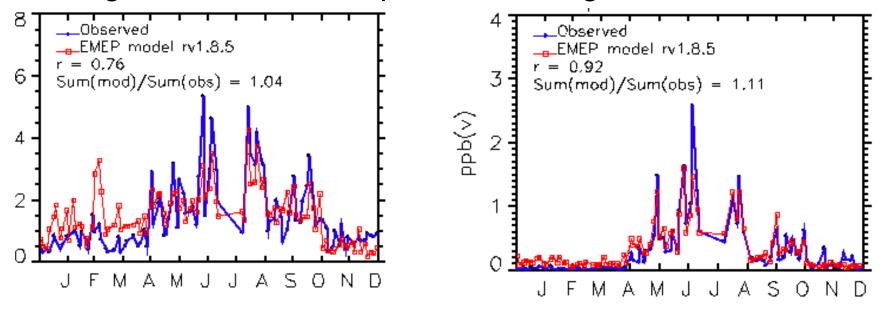
Increase wood OC by factor 3:

Site: KPZ LEVO

r^2(obs vs mod) increases from 0.24 to 0.63!!

Simpler model?

- SOA formation too complex

- Maybe simpler approach just as good?

- Examples:
  - α-pinene + O_x $\Rightarrow$ APIN_OX
  - o-xylene + O_x $\Rightarrow$ OXYL_OX
  - RCHO + O_x $\Rightarrow$ RCHO_OX
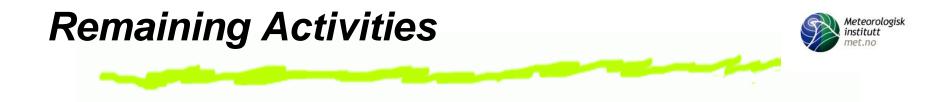 - C5H8 $\Rightarrow$ POLY_ISOP

BSOA?

Too high! Need to check precursors, e.g. Donon, France:

$\Rightarrow$ Evaluation of terpenes needed

Difficulties

- Artefacts ... what do we know?
  - ... reason for summer over-prediction?
  - ... and winter under-prediction?

- Volatility
  - Difficult to account for many compounds in aerosol
  - Aslo compounds such as pinonaldehyde
  - Polymers....

Remaining Activities

- Continue emissions work

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  - Wood-burning

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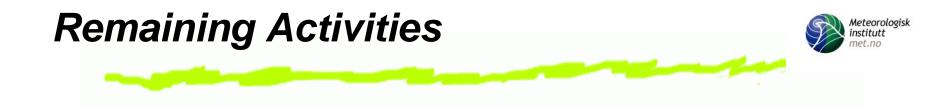
- Revise SOA schemes - simplify ?!!

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- Improve vapour pressure/activity coefficients for OC (UNIFAC)

- Revise SOA schemes - simplify ?!!

- Make use of other compounds - how?!

- Make use of other measurements - e.g. size-distributions

Cont.

- Revise current emission estimates (and uncertainties) for OC anthropogenic and biogenic sources in Europe.
  - Identified important and uncertain source: wood-burning emissions
  - SOA modelling/reconciliation
    - Tools in-place
    - More 'thinking' and analysis needed
  - Need to 'verify' mono-terpenes
- Dynamic modelling
  - (Svetlana Tsyro)
  - Needs emissions by number ... NORPAC?